

MPBP with continuous intermediate variables

Applied to Glauber dynamics

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1 Convolution of tensor trains

Take N probability distributions, each one of a vector of length T of spins $x_i^t \in \{-1, +1\}$, written in tensor train form (can be approximations): $p_i(\bar{x}_i) = A_i^1(x_i^1) A_i^2(x_i^2) \dots A_i^T(x_i^T) \forall i \in 1 \dots N$.

It is wanted to calculate the probability distribution of the variable $h := \sum_{k=1}^N J_k \bar{x}_k$, that is $h^t = \sum_{k=1}^N J_k \bar{x}_k^t \forall t \in 1 \dots T$.¹

$$\begin{aligned} p(y^1, \dots, y^T) &= \sum_{\bar{x}} \prod_i p_i(\bar{x}_i) \prod_t \delta_{y^t, \sum_k J_k x_k^t} = \\ &= \sum_{\bar{x}} \prod_i \prod_t A_i^t(x_i^t) \prod_t \delta_{y^t, \sum_k J_k x_k^t} = \\ &= \sum_{\bar{x}} \prod_i \sum_{\bar{m}_i} \prod_t A_i^t(x_i^t)_{m_i^t, m_i^{t+1}} \prod_t \delta_{y^t, \sum_k J_k x_k^t} = \\ &= \sum_{\bar{x}} \sum_{\bar{m}} \prod_t \left(\delta_{y^t, \sum_k J_k x_k^t} \prod_i A_i^t(x_i^t)_{m_i^t, m_i^{t+1}} \right) = \\ &= \sum_{\bar{m}} \prod_t \sum_{\bar{x}^t} \left(\delta_{y^t, \sum_k J_k x_k^t} \prod_i A_i^t(x_i^t)_{m_i^t, m_i^{t+1}} \right) \end{aligned}$$

Now, the tensors can be expanded in a basis, going from a discrete space to a continuous one. In practice, the elements $A_i^t(x_i^t)_{m_i^t, m_i^{t+1}}$ are written as $\sum_{\alpha} F_i^t[\alpha]_{m_i^t, m_i^{t+1}} u_{\alpha}(x_i^t)$. In the present case, the basis functions u_{α} are chosen to be plane waves with some period P (so that the expansion is a truncated Fourier series): $u_{\alpha}(x) = e^{i \frac{2\pi}{P} \alpha x}$ (see section 2 for more details). Then:

$$p(y^1, \dots, y^T) = \sum_{\bar{m}} \prod_t \sum_{\bar{x}^t} \left(\delta_{y^t, \sum_k J_k x_k^t} \prod_i \sum_{\alpha} F_i^t[\alpha]_{m_i^t, m_i^{t+1}} u_{\alpha}(x_i^t) \right)$$

and promoting the x_i^t s to be continuous variables:

$$p(y^1, \dots, y^T) = \sum_{\bar{m}} \prod_t \int dx_1^t dx_2^t \dots dx_N^t \left(\delta \left(y^t - \sum_k J_k x_k^t \right) \prod_i \sum_{\alpha} F_i^t[\alpha]_{m_i^t, m_i^{t+1}} u_{\alpha}(x_i^t) \right)$$

In order to close the matrix-product ansatz and recover a tensor-train form (expanded in Fourier basis) for $p(y^1, \dots, y^T)$, the following form is sought:

$$\begin{aligned} p(y^1, \dots, y^T) &= \prod_t B^y(y^t) = \sum_{\bar{n}} \prod_t B^t(y^t)_{n^t, n^{t+1}} \\ &= \sum_{\bar{n}} \prod_t \sum_{\gamma} G^t[\gamma]_{n^t, n^{t+1}} u_{\gamma}(y^t) \end{aligned}$$

¹actually, if $x_k^t \in [-P/2, +P/2]$, in order to leave the domain unaltered, the rescaling $x_k^t \mapsto x_k^t/N$ is applied, so that $x_k^t \in [-P/2N, +P/2N]$ and $y^t \in [-P/2, +P/2]$.

It can be easily noticed that:

$$B^t(y^t)_{n^t, n^{t+1}} = \int dx_1^t dx_2^t \dots dx_N^t \left(\delta \left(y^t, \sum_k J_k x_k^t \right) \prod_i \sum_\alpha F_i^t[\alpha]_{m_i^t, m_i^{t+1}} u_\alpha(x_i^t) \right)$$

where the index n^t is actually a multi-index $n^t = (m_1^t, m_2^t, \dots, m_N^t)$.

Then, in the case of $N = 2$ tensors (which is the recursive step that allows to calculate all the others):

$$\begin{aligned} B^t(y^t)_{(m_1^t, m_2^t), (m_1^{t+1}, m_2^{t+1})} &= \int dx_1^t \int dx_2^t \left[\delta(y^t - J_1 x_1^t - J_2 x_2^t) \left(\sum_\alpha F_1^t[\alpha]_{m_1^t, m_1^{t+1}} u_\alpha(x_1^t) \right) \left(\sum_\beta F_2^t[\beta]_{m_2^t, m_2^{t+1}} u_\beta(x_2^t) \right) \right] = \\ &= \sum_{\alpha, \beta} F_1^t[\alpha]_{m_1^t, m_1^{t+1}} F_2^t[\beta]_{m_2^t, m_2^{t+1}} \int dx_1^t \int dx_2^t \delta(y^t - J_1 x_1^t - J_2 x_2^t) u_\alpha(x_1^t) u_\beta(x_2^t) \end{aligned}$$

And then it is easy to find the coefficients of the basis expansion:

$$\begin{aligned} G^t[\gamma]_{(m_1^t, m_2^t), (m_1^{t+1}, m_2^{t+1})} &= \frac{1}{P} \int B^t(y^t)_{(m_1^t, m_2^t), (m_1^{t+1}, m_2^{t+1})} u_\gamma^*(y^t) dy^t = \\ &= \frac{1}{P} \sum_{\alpha, \beta} F_1^t[\alpha]_{m_1^t, m_1^{t+1}} F_2^t[\beta]_{m_2^t, m_2^{t+1}} \int dx_1^t \int dx_2^t \int dy^t [\delta(y^t - J_1 x_1^t - J_2 x_2^t) u_\alpha(x_1^t) u_\beta(x_2^t) u_\gamma^*(y^t)] = \\ &= \frac{1}{P} \sum_{\alpha, \beta} F_1^t[\alpha]_{m_1^t, m_1^{t+1}} F_2^t[\beta]_{m_2^t, m_2^{t+1}} \int dx_1^t \int dx_2^t [u_\alpha(x_1^t) u_\beta(x_2^t) u_\gamma^*(J_1 x_1^t + J_2 x_2^t)] \end{aligned}$$

All that remains is to calculate the double integral:

$$\begin{aligned} I_{\alpha, \beta, \gamma} &= \frac{1}{P} \int dx_1^t \int dx_2^t [u_\alpha(x_1^t) u_\beta(x_2^t) u_\gamma^*(J_1 x_1^t + J_2 x_2^t)] = \\ &= \frac{1}{P} \int dx_1 e^{i \frac{2\pi}{P} (\alpha - J_1 \gamma) x_1} \int dx_2 e^{i \frac{2\pi}{P} (\beta - J_2 \gamma) x_2} = \\ &= \frac{1}{P} \left(-\frac{iP}{2\pi(\alpha - J_1 \gamma)} \left[e^{i \frac{2\pi}{P} (\alpha - J_1 \gamma) x_1} \right]_{x_1=-s_1}^{x_1=s_1} \right) \cdot \left(-\frac{iP}{2\pi(\beta - J_2 \gamma)} \left[e^{i \frac{2\pi}{P} (\beta - J_2 \gamma) x_2} \right]_{x_2=-s_2}^{x_2=s_2} \right) = \\ &= \frac{4}{P} \frac{\sin(\frac{2\pi}{P}(\alpha - J_1 \gamma)s_1)}{\frac{2\pi}{P}(\alpha - J_1 \gamma)} \cdot \frac{\sin(\frac{2\pi}{P}(\beta - J_2 \gamma)s_2)}{\frac{2\pi}{P}(\beta - J_2 \gamma)} \end{aligned}$$

Then the desired form is recovered:

$$G^t[\gamma]_{(m_1^t, m_2^t), (m_1^{t+1}, m_2^{t+1})} = \sum_{\alpha, \beta} F_1^t[\alpha]_{m_1^t, m_1^{t+1}} F_2^t[\beta]_{m_2^t, m_2^{t+1}} I_{\alpha, \beta, \gamma}$$

and one can calculate the convolution with all the N terms in a recursive way, by taking the right s_1 and s_2 . The only problem is that, at each iteration, the sizes of the tensors grow, rendering this approach of exponential complexity in N . This can be solved by applying, at each iteration, two sweeps of SVD and truncation to the tensors $G^t[\gamma]$, reducing and controlling their sizes.

2 Calculation of coefficients

One has a probability distribution for a spin: $p(x) = p(-s_1)\delta_{x, -s_1} + p(+s_1)\delta_{x, +s_1}$ and wants to compute its Fourier series coefficients. Thus, the distribution can be approximated with a sum of Gaussian, each with small variance σ^2 , as depicted in Figure 1:

$$f(x) \simeq \frac{1}{\sqrt{2\pi}\sigma^2} \left(p(-s_1)e^{-\frac{(x+s_1)^2}{2\sigma^2}} + p(+s_1)e^{-\frac{(x-s_1)^2}{2\sigma^2}} \right)$$

The coefficients of the Fourier series can then be calculated as scalar products with the basis functions:

$$\begin{aligned} C_\alpha &= \frac{1}{P} \int_{-P/2}^{+P/2} f(x) u_\alpha^*(x) dx = \frac{1}{P} \int_{-P/2}^{+P/2} \frac{1}{\sqrt{2\pi}\sigma^2} \left(p(-s_1)e^{-\frac{(x+s_1)^2}{2\sigma^2}} + p(+s_1)e^{-\frac{(x-s_1)^2}{2\sigma^2}} \right) e^{i \frac{2\pi}{P} \alpha x} dx \simeq \\ &\simeq \frac{1}{P\sqrt{2\pi}\sigma^2} \left(p(-s_1) \int_{-\infty}^{+\infty} e^{-\frac{(x+s_1)^2}{2\sigma^2} - i \frac{2\pi}{P} \alpha x} dx + p(+s_1) \int_{-\infty}^{+\infty} e^{-\frac{(x-s_1)^2}{2\sigma^2} - i \frac{2\pi}{P} \alpha x} dx \right) \end{aligned}$$

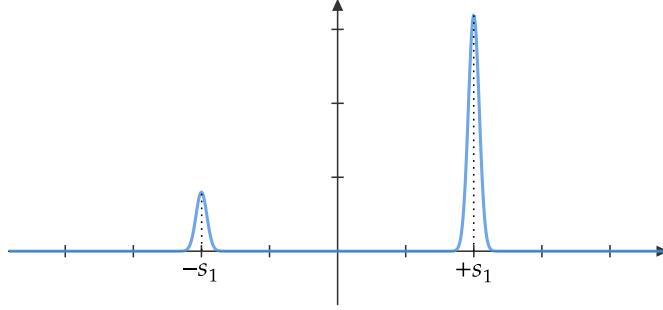


Figure 1: Approximation of the pdf of a spin as a sum of two Gaussians.

The integrals are easily calculated by completing the squares in the exponents:

$$\int_{-\infty}^{+\infty} e^{-\frac{(x \pm s_1)^2}{2\sigma^2} - i \frac{2\pi}{P} \alpha x} dx = \sqrt{2\pi\sigma^2} e^{-\frac{2\pi^2}{P^2}\sigma^2\alpha^2} \left[\cos\left(\frac{2\pi}{P}\alpha s_1\right) \pm i \sin\left(\frac{2\pi}{P}\alpha s_1\right) \right]$$

$$\begin{aligned} C_\alpha &= \frac{e^{-\frac{2\pi^2}{P^2}\sigma^2\alpha^2}}{P} \left[p(-s_1) \left(\cos\left(\frac{2\pi}{P}\alpha s_1\right) + i \sin\left(\frac{2\pi}{P}\alpha s_1\right) \right) + p(+s_1) \left(\cos\left(\frac{2\pi}{P}\alpha s_1\right) - i \sin\left(\frac{2\pi}{P}\alpha s_1\right) \right) \right] = \\ &= \frac{e^{-\frac{2\pi^2}{P^2}\sigma^2\alpha^2}}{P} \left[(p(-s_1) + p(s_1)) \cos\left(\frac{2\pi}{P}\alpha s_1\right) + i(p(-s_1) - p(s_1)) \sin\left(\frac{2\pi}{P}\alpha s_1\right) \right] = \\ &= \frac{e^{-k_\alpha^2\sigma^2}}{P} [(p(-s_1) + p(s_1)) \cos(k_\alpha s_1) + i(p(-s_1) - p(s_1)) \sin(k_\alpha s_1)] \end{aligned}$$

having defined $k_\alpha := \frac{2\pi}{P}\alpha$.

3 Belief Propagation message update

The BP update equations are to be written using the tensor-train approximation and the decomposition on a Fourier basis.

$$\begin{aligned} \mu_{i \rightarrow j}(\bar{x}_i, \bar{x}_j) &= \sum_{\{\bar{x}_k\}_{k \in \partial i \setminus j}} \prod_t \omega\left(x_i^{t+1}, \sum_{k \in \partial i} J_{ki} x_k^t\right) \prod_{k \in \partial i \setminus j} \mu_{k \rightarrow i}(\bar{x}_k, \bar{x}_i) = \\ &= \sum_{\{\bar{x}_k\}_{k \in \partial i \setminus j}} \int dy^0 \cdots \int dy^T \prod_t \omega(x_i^{t+1}, y^t + J_{ji} x_j^t) \delta\left(y^t - \sum_{k \in \partial i \setminus j} J_{ki} x_k^t\right) \prod_{k \in \partial i \setminus j} \mu_{k \rightarrow i}(\bar{x}_k, \bar{x}_i) = \\ &= \int \cdots \int \prod_t dy^t \prod_t \omega(x_i^{t+1}, y^t + J_{ji} x_j^t) \underbrace{\sum_{\{\bar{x}_k\}_{k \in \partial i \setminus j}} \prod_t \delta\left(y^t - \sum_{k \in \partial i \setminus j} J_{ki} x_k^t\right)}_{\text{this is a convolution of the type described in section 1}} \prod_{k \in \partial i \setminus j} \mu_{k \rightarrow i}(\bar{x}_k, \bar{x}_i) = \\ &= \int \cdots \int \prod_t dy^t \prod_t \omega(x_i^{t+1}, y^t + J_{ji} x_j^t) \prod_t B^t(y^t, x_i^t) = \\ &= \prod_t \int dy^t \omega(x_i^{t+1}, y^t + J_{ji} x_j^t) \sum_{\gamma^t} G^t[\gamma^t, x_i^t] u_{\gamma^t}(y^t) \end{aligned}$$

Then, for each time:

$$\tilde{A}^t(x_i^{t+1}, x_i^t, x_j^t) = \int dy^t \omega(x_i^{t+1}, y^t + J_{ji} x_j^t) \sum_{\gamma^t} G^t[\gamma^t, x_i^t] u_{\gamma^t}(y^t)$$

where the calculation has to be performed for each and every matrix element:

$$\begin{aligned} \left[\tilde{A}^t(x_i^{t+1}, x_i^t, x_j^t) \right]_{n^t, n^{t+1}} &= \int dy^t \omega(x_i^{t+1}, y^t + J_{ji}x_j^t) \sum_{\gamma^t} [G^t[\gamma^t, x_i^t]]_{n^t, n^{t+1}} u_{\gamma^t}(y^t) = \\ &= \sum_{\gamma^t} [G^t[\gamma^t, x_i^t]]_{n^t, n^{t+1}} \int dy^t \omega(x_i^{t+1}, y^t + J_{ji}x_j^t) u_{\gamma^t}(y^t) = \\ &= \sum_{\gamma^t} [G^t[\gamma^t, x_i^t]]_{n^t, n^{t+1}} I_{\gamma^t}(x_i^{t+1}, x_j^t) \end{aligned}$$

The indefinite integral can be calculated as follows²:

$$\begin{aligned} I_{\gamma^t}(x_i^{t+1}, x_j^t) &= \int dy^t \omega(x_i^{t+1}, y^t + J_{ji}x_j^t) u_{\gamma^t}(y^t) = \\ &= \int dy^t \frac{e^{\beta(y^t + J_{ji}x_j^t + h_i)x_i^{t+1}}}{2 \cosh(\beta(y^t + J_{ji}x_j^t + h_i))} e^{i \frac{2\pi}{P} \gamma^t y^t} = \\ &= \frac{e^{ik_\gamma y^t}}{\beta(1 + x_i^{t+1}) + ik_\gamma} e^{\beta(y^t + J_{ji}x_j^t + h_i)(1 + x_i^{t+1})} {}_2F_1 \left(1, \frac{\beta(1 + x_i^{t+1}) + ik_\gamma}{2\beta}, \frac{\beta(3 + x_i^{t+1}) + ik_\gamma}{2\beta}, -e^{2\beta(y^t + J_{ji}x_j^t + h_i)} \right) \end{aligned}$$

and the extrema for calculating the definite integral are $y^t = -d_i + 1$ and $y^t = d_i - 1$, respectively.

If $x_i^{t+1} = -1$ and $\gamma = 0$ the integral can be easily calculated to be:

$$I_0(-1, x_j^t) = \int dy^t \frac{e^{-\beta(y^t + J_{ji}x_j^t + h_i)}}{e^{\beta(y^t + J_{ji}x_j^t + h_i)} + e^{-\beta(y^t + J_{ji}x_j^t + h_i)}} = -\frac{1}{2\beta} \log \left(1 + e^{-2\beta(y^t + J_{ji}x_j^t + h_i)} \right)$$

The final sought form is $\mu_{i \rightarrow j}(\bar{x}_i, \bar{x}_j) = \prod_t A(x_i^t, x_j^t)$. In the previous form, the variables x_i^{t+1} and x_i^t were coupled in the same tensor \tilde{A}^t . To solve this, a sweep of SVD is sufficient.

4 Calculation of beliefs

The calculations are essentially the same as those performed in section 3 for the messages. The only difference is that the convolution is performed on all $\mu_{k \rightarrow i} \forall k \in \partial i$ and that the summation is performed on $\{\bar{x}_k\}_{k \in \partial i}$. These facts have the effect that the integral $I_{\gamma^t}(x_i^{t+1}, x_j^t)$ does not depend on x_j^t , so one can formally define a new integral $I'_{\gamma^t}(x_i^{t+1}) := I_{\gamma^t}(x_i^{t+1}, x_j^t = 0)$. Then the beliefs can be computed:

$$b_i(\bar{x}_i) = \prod_t C^t(x_i^t)$$

where the matrices C^t are obtained by means of a sweep of SVD from:

$$\tilde{C}^t(x_i^t) = \sum_{\gamma^t} G^t[\gamma^t, x_i^t] I'_{\gamma^t}(x_i^{t+1})$$

with G^t being the matrices resulting from the convolution of all the incoming messages in i .

²This has been done by Wolfram Mathematica with the input `Integrate[1/2 Exp[b (y + J) x]/Cosh[b (y + J)] Exp[I k y], y, Assumptions -> {b \in Reals, J \in Reals, x \in Reals, k \in Reals, y \in Reals}]`.